Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.53e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.30e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

Image not found
1-Hexanol
Measured: 5.77e-02
Predicted: 5.53e-02

Image not found
4-Methylpentan-1-ol
Measured: 7.34e-02
Predicted: 5.57e-02

Image not found
3-Methyl-1-pentanol
Measured: 4.21e-02
Predicted: 5.25e-02

Image not found
2-Methyl-1-pentanol
Measured: 5.87e-02
Predicted: 7.88e-02

Image not found
2-Ethyl-1-butanol
Measured: 3.91e-02
Predicted: 7.91e-02